



# Inverse modeling of indoor instantaneous airborne contaminant source location with adjoint probability-based method under dynamic airflow field



Haidong Wang<sup>a,\*</sup>, Sai Lu<sup>a</sup>, Jiajia Cheng<sup>a</sup>, Zhiqiang (John) Zhai<sup>b</sup>

<sup>a</sup> School of Environment and Architecture, University of Shanghai for Science and Technology, 516 Jungong Road, Shanghai, 200093, PR.China

<sup>b</sup> Department of Civil, Environmental and Architectural Engineering, University of Colorado Boulder, 428UCB, Boulder, 80309-0428, CO, USA

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## ABSTRACT

Accurate and prompt identification of airborne contaminant source location in indoor environment is of vital importance for building operation safety. Successful inverse tracking algorithm to identify airborne contaminant location usually requires limited sensor readings and indoor airflow information as input. Such mathematical algorithm under steady-state indoor airflow scenario has been intensively investigated. However, in many built environment scenarios, air velocity direction and magnitude keeps changing with time, making the transportation process of airborne contaminant significantly different from it under steady-state airflow. This paper mainly focuses on the airborne contaminant source location identification under dynamic airflow, by employing an adjoint probability-based inverse tracking method. The mathematical model and process of indoor instantaneous contaminants source location identification under dynamic air flow field is investigated and presented. Case studies using Computational Fluid Dynamics (CFD) tool by unsteady RANS simulation are conducted on a subway station model as well as an aircraft cabin, in which case experimental validation is also conducted. The capability of the new method is verified for air contaminant source location identification under dynamic indoor airflow.

**Practical implications:** Successful identification of airborne contaminant source location under dynamic airflow field implies the capability of the method to locate an airborne contaminant source by limited sensor information and time-dependent airflow field in real-time. Practically the time-dependent airflow field data can be obtained through CFD simulation with unsteady RANS model with monitored time-dependent boundary condition.

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## 1. Introduction

Indoor airborne contaminant received great attention recent years for indoor environment quality (IEQ) concern and building safety issue. When a certain concentration of toxic airborne contaminant was released into enclosed spaces, the contamination will quickly spread to the entire space and cause serious consequences. Therefore, prompt and accurate identification of airborne contaminant source characteristics will greatly assist isolation and removal of the source, therefore diminishes the consequence of such incidence effectively. Such process of identifying the source

releasing location and possibly releasing time by limited sensor reading is a typical inverse problem.

Inverse problems are common and widely investigated in various applications, such as inverse modeling of the atmospheric pollution to identify the location [1–4] and releasing rate [5,6] of air pollutant source, diffusion of carbon monoxide concentrations in forest fires to deal with sudden accidents [7], and design of aircraft cabin environment [8]. In typical built environment, airborne contaminant transports with airflow through convection and diffusion, therefore airflow field information is indispensable part of input data for such algorithms. A sensor system providing concentration readings is another input for the model. Algorithms and case studies of identifying indoor airborne contaminant have been well established under different scenarios following such ideology.

Zhai categorized inverse tracking problem to three main types

\* Corresponding author.

E-mail address: [whd@usst.edu.cn](mailto:whd@usst.edu.cn) (H. Wang).

[9], which are forward method [10–12], reverse method [9,13,14], and probability calculation method [15]. The forward method usually requires large amount of computation to trial all possible source and its consequences and therefore time-consuming. It diminishes the role of inverse modeling in the real-time identification of source location. To overcome such disadvantages, Sohn used Bayesian statistics to interpret the pollutant concentrations from several sensors which were installed in the building, and then computed the best uncertainties conditions of the pollutant source [16]. Bayesian probability theory was employed to identify the gaseous pollutant source by interpreting real-time monitoring information [17,18]. An artificial neural network based method working with multi-zone model is an alternative for speed purpose [19,20]. Cai and Li [21,22] conducted pollutants real-time positioning of pollutants releasing at a constant speed and multiple sources by a linear programming model built on an analytical expression of indoor contaminant dispersion.

Two typical backward inverse methods named quasi-reversibility(QR) and pseudo-reversibility(PR) were proposed to study the localization of gaseous [23] and particulates [24] pollutants released by steady and unsteady pollutant source in an enclosed cabin [25]. Zhang extended QR to Lagrangian-reversibility(LR) method [26] for particle tracking and improved the accuracy of the backward inverse method. Besides, Zhang also employed an inverse method based on Tikhonov regularization and least-squares optimization to calculate the mass of the pollutant [27] and then proposed an inverse matrix submodel to inversely determine the temporal release rate profile and a Bayesian probability submodel to identify its releasing location and the corresponding sensor alarming time [28].

Liu and Zhai used probability algorithm to identify location of the instantaneous [29,30] and dynamic [29] indoor contaminant source, and such probability-based inverse multi-zone model was utilized to successfully track contaminant source location with known source releasing time in a multi-zonal building. This method is proved to be successful in assisting the design of a high-performance sensors network system and identifying contaminant source locations for an entire building based on limited sensors [15].

Most, if not all, of the previous studies mentioned assumed steady-state indoor/outdoor airflow field during releasing of airborne contaminant source. Such airflow field information, obtained by measurement or through computer modeling, is one of the key input parameters for these problems. In the real case scenarios, however, air velocity and temperature may change at any time in instances such as variable air volume system (VAV) and natural ventilation environment. In certain special cases airflow field changes periodically with time. This imposes a great challenge for contaminant source identification method of previous studies.

In this paper, a mathematical model and process for identifying an instantaneous airborne contaminant location under dynamic airflow indoor environment is developed and investigated based on the well-established adjoint probability method. The indoor airflow field information obtained from time-dependent computational fluid dynamics (CFD) simulation is utilized. Limited sensor readings are used as input parameter. Case studies with typical dynamic airflow conditions verify the capability of such model and process in application of time-dependent/dynamic airflow field circumstance.

## 2. Methods

### 2.1. Principles of probability-based inverse modeling method

Probability method of inverse modeling is used to estimate the

probability of an event as a target probabilistic function, through the maximum or minimum and the objective function to find out the information of the source. Neupauer and Wilson [31,32] developed a method to predict water pollutant source location and travel time probabilities in the earlier years. Because of the similar spreading characteristics of pollutants in water and air, Liu and Zhai [9] extended this method and applied it to indoor environment to identify the potential indoor pollutant source characteristics with limited sensor readings. This method has been intensively validated for steady-state airflow field scenario.

With a focus on unsteady airflow field, in which instantaneous indoor air contaminant sources location is identified, this paper extends the adjoint probability method for the application of time-dependent airflow field. The basic principle and the corresponding probability equations of the adjoint probability method based on CFD are introduced below.

### 2.2. Fundamentals of adjoint probability method under dynamic airflow

Assume that there is an instantaneous point contaminant source of a total mass  $M_0$  in an enclosed environment at certain position of  $\vec{x} = \vec{x}_0$ , which releases the contaminant into the air at time  $t=0$ . The contaminant will spread to the entire space in a finite time. At  $t = T > 0$ , any location in the enclosed environment can be considered as the potential source of contamination as long as the contaminant through the air flow reaches it, and the probability of the potential contaminant source is defined as the forward location probability [33–35]. For example, the contaminant source though the air flow spread to the finite volume  $\Delta V_1$  at the position of  $\vec{x} = \vec{x}_1$  is  $M_1$  when  $t = T$ , the forward location probability at the position of  $\vec{x} = \vec{x}_1$  at time  $t = T$  can be expressed as Eq. (1).

$$P(\Delta V_1 | \vec{x} = \vec{x}_1, t = T, \vec{x}_0) = \frac{M_1}{M_0} \quad (1)$$

Using  $f_x$  to represent the per volume probability value, this equation can be expressed as:

$$f_x(\vec{x}, t = T, \vec{x}_0) = \frac{P(\Delta V_1 | \vec{x} = \vec{x}_1, t = T, \vec{x}_0)}{\Delta V_1} = \frac{M_1}{M_0} / \Delta V_1 = \frac{C_1}{M_0} \quad (2)$$

In Eq. (2),  $C_1$  represents the concentration value of the contaminant at  $\vec{x} = \vec{x}_1$ . A general format of Eq. (2) is:

$$f_x(\vec{x}, t = T, \vec{x}_0) = \frac{C(\vec{x}, T)}{M_0} \quad (3)$$

In Eq. (3),  $f_x(\vec{x}, t = T, \vec{x}_0)$  represents the probability that certain position being the potential contaminant source at  $t = T$ ,  $\vec{x}$  is random position in the enclosed environment,  $C(\vec{x}, T)$  represents the concentration value of contaminant at  $t = T$  due to the release of the instantaneous point contaminant source. The right side of Eq. (3) is the ratio of such concentration to the total released mass at position of  $\vec{x}_0$ , therefore can be generalized as  $\frac{dC(\vec{x}, T)}{dM_0}$ . Using  $\psi_x(\vec{x}, t = T, \vec{x}_0)$  to represent such ratio will lead to:

$$f_x(\vec{x}, t = T, \vec{x}_0) = \frac{dC(\vec{x}, T)}{dM_0} = \psi_x(\vec{x}, t = T, \vec{x}_0) \quad (4)$$

The forward location probability density function  $f_x(\vec{x}, t = T, \vec{x}_0)$  can be interpreted as the probability of an instantaneous point contaminant source at the location of  $\vec{x}_0$ , spreading

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